Analysis of Interfacial Properties for Water, Co_2 and Hydrocarbon Systems Using Density Functional Theory

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We present in this work a qualitative and quantitative study of several interfacial and surface phenomena based on density functional theory. A theoretical analysis is needed due to lack of experimental capabilities to determine properties of inhomogeneous fluids such us density profiles, surface/interfacial tension, adsorption, and solvation forces. The density functional theory treatment used for this report is embedded in *Tramonto*, software developed by Sandia National Laboratories. Interfacial tension calculations have been developed for hydrocarbon in the series from C_1 to C_{10}, CO_2 and water and compared to experimental data. Binary system containing CO_2 and hydrocarbon were also studied using a fundamental approach based upon hard core interactions combined with Lennard Jones potentials. A consistent pattern was found for all the analyzed systems, good agreement in the interfacial density predictions does not guarantee a good agreement for the liquid densities determination and vice versa. Finally binary systems for water, hydrocarbons and CO_2 were analyzed. In this case considerable differences were found between experimental and predicted values due to lack of a comprehensive and physically consistent model for representing water interactions including association in Tramonto.